

HEAT AND MASS TRANSFER MODELLING IN LYOPHILIZATION PROCESS FOR AN APPLE SLICES

VIKAS GARG¹, P. SUDHAKAR RAO² & HARRY GARG³

^{1,2}Department of Mechanical Engineering, National Institute of Technical Teachers Training and Research, Chandigarh, India

³Precision Mechanical Systems, Central Scientific Instruments organization (CSIR-CSIO), Chandigarh, India

ABSTRACT

The aim of this paper is to develop a mathematical model, which simulates the lyophilization process for an apple slices. In the lyophilization process, the moisture content in the slices is removed with the help of a freeze drying process, the whole process results in the preservation of the food materials by increasing their shelf life, stability and by reducing the spoilage. So as to achieve this aim, a numerical analysis has been performed by developing a mathematical model on COMSOL 5.3a software on a HP Z840 workstations, which solves the different equations involved in the heat and mass transfer mechanism for the drying of an apple slices. The Comsol Multiphysics software helps to couple the heat transfer and mass transfer simultaneously involved in the process. The modeling of freeze drying process is a challenging task because of variable thermal properties of the material w.r.t temperature and moisture content are involved. The developed simulation is confined to the heat and mass transfer behavior of an apple slice, irrespective to the effect on biological aspect such as tissues inside the apple during the freeze drying, and it is only capable to predict the temperature and moisture content in the entire slice. This prediction helps to optimize the process parameters such as target temperature, drying rate for the process. The developed simulated model is a great tool to analyze the behavior of the drying process, and the developed model is too flexible that it can be applied to other varieties of fruits by changing their thermal properties.

KEYWORDS: Lyophilization, Freeze Drying, Heat and Mass transfer Simulation, Mathematical Model & Sublimation

Received: Apr 25, 2019; **Accepted:** May 16, 2019; **Published:** Jun 24, 2019; **Paper Id.:** IJMPERDAUG201928

1. INTRODUCTION

Lyophilization is a dehydration process, which often used to preserve putrescible food or materials. It improves the long term stability of work. It is a three steps process of removing most of the total moisture content from the material. The three steps are interdependent. The first step is to freeze the material, followed by lowering the surrounding pressure to a level, where frozen material starts to sublime. At the end of this stage second step begins, represented by sublimation of ice. This step is also called as primary drying. At this stage, almost 90% of the material moisture is removed. As the sublimation ends, the third step, which is also called secondary drying starts. In this stage, desorption takes place for bounded water molecules in the dried material.

Freeze drying results in a good quality of product, due to the low temperature used in the processing. The existing shape of the product remains same and the quality of the re-hydrated product is extremely good [1].

Heat and mass transfer across the interfaces is very important in food processing mechanisms. In other words, food processing is about to creating, preserving and manipulating the food structures. Drying plays an important role in preserving the food and to maintain its appearance, original taste this task is very challenging.

Nowadays, this drying process is used on a large scale, so as to produce more desirable foods and to preserve the foods [2]. Due to high costs involved in the lyophilization process, many researchers focussed on its study and design space [3].

A model is a replica of real problem and for its representation, a mathematical model is used. This developed model is significantly used in design and optimization purpose. The main features of the process in this paper are its ability to predict temperature and moisture in the entire material, which is important way to optimize the different parameters. The aim is to make all the details for the process as possible, without creating unnecessary computational complexity or time commitment. Therefore, it is necessary, in process engineering area to model and interpret the behavior and the characteristics of the system under study [4].

Moisture content and temperature are the most important factors in the conservation of fruits [5]. The metabolism in food is accelerated when the temperature of the material is high. In the entire process, heat and mass transfer plays important, which involves nonlinear behavior when freezing and drying processes are involved; many researchers have focused on developing a physical model and on numerical techniques, so as to solve them as can be found in scientific literature [6]. Thermal properties, like specific heat of the material and thermal conductivity, shows sudden changes near the freezing point and gives nonlinear partial differential relations that are difficult to analyze. The behavior of freezing and drying can be difficult to predict in case of complex shapes of the objects. So as to govern these practical processes, it requires numerical solution [7].

2. GOVERNING EQUATIONS

The equations involved in freeze drying process are applied only for the volume of material. The material is assumed to be homogeneous. At the beginning of the process, the entire volume is considered as frozen part, as the process progresses the moisture content in the upper part will start to sublime.

2.1 Conservation of Energy

The equation of heat conservation can be written as in equation 1: [8]

$$\rho \left\{ \frac{\partial (C_p T)}{\partial t} + \vec{\nabla} (C_p T) \right\} = \vec{\nabla} (k \vec{\nabla} T) \quad (1)$$

2.2 Conservation of Mass

The equation of mass conservation can be written as in equation 2: [9]

$$\rho \left\{ \frac{\partial M}{\partial t} + \vec{\nabla} M \right\} = \vec{\nabla} (\rho D \vec{\nabla} M) \quad (2)$$

In the secondary drying stage, the equation 3 can be used to determine the rate of desorption the drying kinetics model of first order [10].

$$\frac{\partial C}{\partial t} = k_g (C^* - C) \quad (3)$$

Where k_g represents the mass transfer coefficient and C^* the equilibrium water concentration, which depends on the partial pressure of the water vapour, the amount of bounded water inside the dried material and temperature.

Table 1: Nomenclature

Units	Description
ρ	Density [kg/m ³]
M	Moisture content [dry basis]
R_0	Radius of the slice [mm]
H_0	Height of the slice [mm]
M_0	Initial moisture content
k	Thermal conductivity[W/m*K]
T	Temperature [K]
C^*	Equilibrium concentration [-]
C	Concentration [-]
T_0	Initial temperature [K]

3. COMPUTATIONAL MODEL

Simulation of drying of an apple was performed in COMSOL 5.3a using finite element analysis, which compute the drying behavior of an apple slices. The heat and mass transfer equations are solved in the software. The software includes all the steps for modeling process starting from creating geometry, defining parameters and variables, specifying physics, meshing and then visualizes the results. The COMSOL software was very useful in variable thermal properties of material, where the properties vary with the temperature and the moisture content. The software couples the heat and mass transfer equations, simultaneously. The simulation, models the temperature and moisture distribution inside the material during freeze drying. The software solves the heat and mass transfer equations with the time dependent interface.

3.1 Mode Definition

A 2D axisymmetric geometry was created in the software as shown in the figure 1. The figure shows quarterly part of the geometry, which helps the software to reduce the computational time.

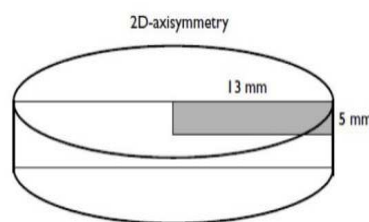


Figure 1: Geometry of an Apple Slice

The simplifications in the axisymmetric model give a 2D view in a rectangular domain as shown in the figure 2

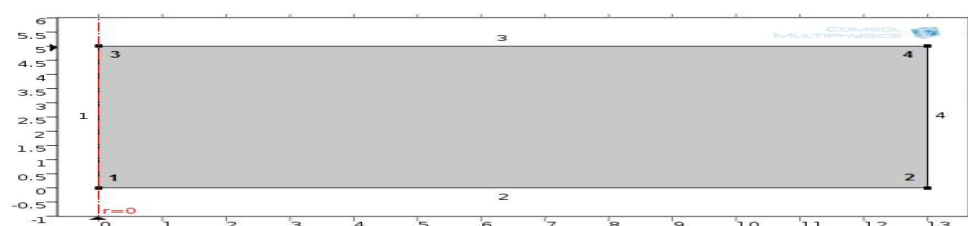


Figure 2: Model Domain and Boundaries

Boundary Conditions

The vaporization of water takes place from the upper part of the slice. So, the boundary conditions are needed to apply on the model so that a defined heat flux can take place.

The model has following dimensions:

The diameter and height of a slice is 26 mm and 10 mm, respectively. The heat flux is represented by $D\lambda \nabla C$ for the boundaries 3 and 4. The axisymmetric about the axis is represented by boundary 1 and temperature symmetry is represented by boundary 2.

Initial boundary conditions:

At the beginning of the process, the initial boundary conditions for the moisture content and temperature are shown in equation no.4 and 5:

$$M = M_0 \quad (4)$$

$$T = T_0 \quad (5)$$

Due to symmetry, the moisture content and the temperature gradients are zero at the center. So, the boundary conditions are shown in equation no.6:

$$\frac{\partial M}{\partial X} = 0 \text{ And } \frac{\partial T}{\partial X} = 0 ; \text{ At } X = 0 \quad (6)$$

At the surface, the heat flux out from the slice on the boundary 3 and 4 due to the vaporization of moisture content are shown in equation no. 7 and 8[8]:

$$n.(-k \nabla T) = 0 ; \text{ At boundary 1 and 2} \quad (7)$$

$$n.(-k \nabla T) = h_T (T_{air} - T) + \lambda (D \nabla C) ; \text{ At boundary 3 and 4} \quad (8)$$

The boundary conditions for the diffusion process are written in equation 9 and 10:

$$n.(-D \nabla C) = 0 ; \text{ At boundary 1 and 2} \quad (9)$$

$$n.(-D \nabla C) = k_c (C^* - C) ; \text{ At boundary 3 and 4} \quad (10)$$

The boundaries and domain of the computational model is shown in the figure 3, in which homogenous heat flux was represented in the Comsol software [11].

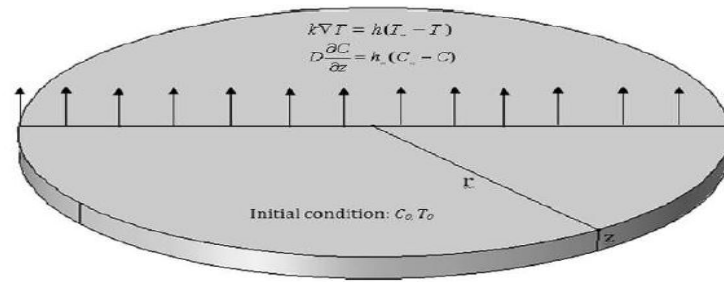


Figure 3: Computational Model Representing Heat Flux [11]

The meshing of the model was created for a rectangular domain as discussed in the previous section. The triangular meshing was created near the boundary 3 and 4 with maximum element size of 0.1 and for the remaining part the extra fine meshing was created as shown in the figure 4.

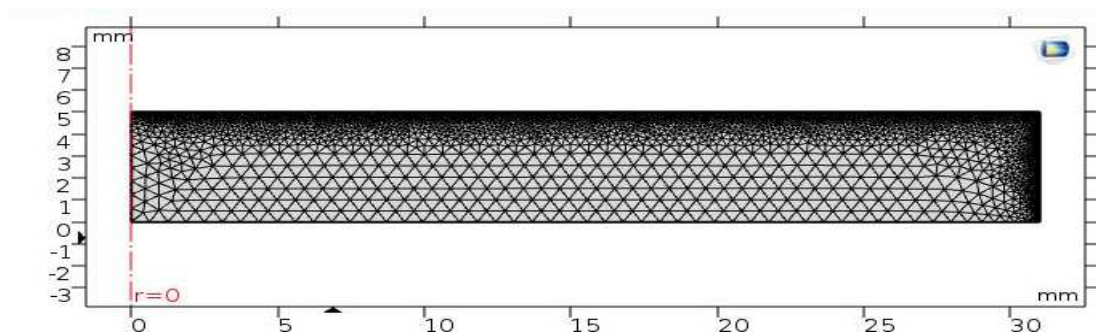


Figure 4: Meshing of the Rectangular Domain

The input parameters of the computed model used in the simulation of drying process are shown in the table 2. The temperature of the chamber was kept at 272.15 K, and the initial temperature of the slice was 248.15 K. The thermal conductivity and specific heat of the material depends on the temperature and moisture concentration in the material [11].

Some researchers proposed the relation of the thermal properties of food materials with the moisture content [12].

The thermal conductivity varies with the moisture content can be written as shown in equation 11:

$$k = 0.148 + 0.00493 * (\% \text{ moisture}) \quad (11)$$

Table 2: Parameters and their Values used in the Model

Parameters	Symbol	Value
Chamber temperature	T _{air}	272.15 [K]
Initial temperature	T ₀	248.15 [K]
Density of material	rho _s	788 [kg/m ³]
Water molecular weight	M _{H₂O}	18 [g/mol]
Initial concentration	C ₀	0.873
Diffusion coefficient	D	3.3*10 ⁻⁹ [m ² /s]

4. RESULTS AND DISCUSSIONS

The drying kinetics of an apple slice was solved in comsol 5.3a. The temperature and moisture contents were observed under time domain in the software.

Figure 5 & 6 shows moisture transport w.r.t time, respectively.

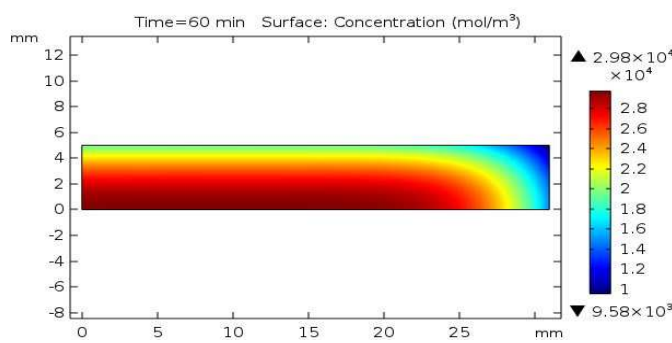


Figure 5: Moisture Transports after 1 hr

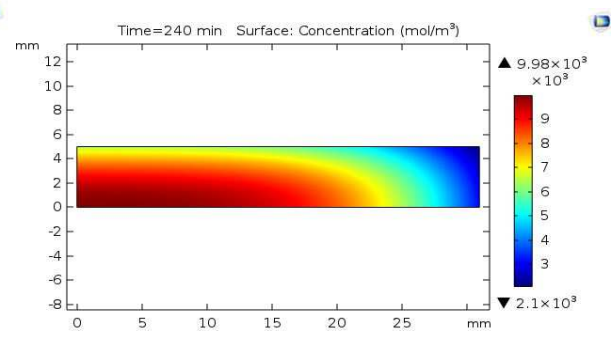


Figure 6: Moisture Transports after 4 hrs

The above figures show, the moisture content decreases with the progress of time. Initially, there was 87.3 % moisture content in the slice, to reduce the moisture content up to a certain value in a particular temperature range; this model helps to give time required for an apple slice to reach a certain value. The data is shown in the table 3 which shows the time required for an apple slice to achieve the moisture content 75%, 50%, 25%, 5%, respectively.

Table 3: Shows Time Taken to Reach Desired Moisture Content

S. No.	Moisture content	Time (min)
1	75%	15
2	50%	62
3	25%	151
4	5%	382

Figure 7 & 8 shows temperature distribution w.r.t time respectively.

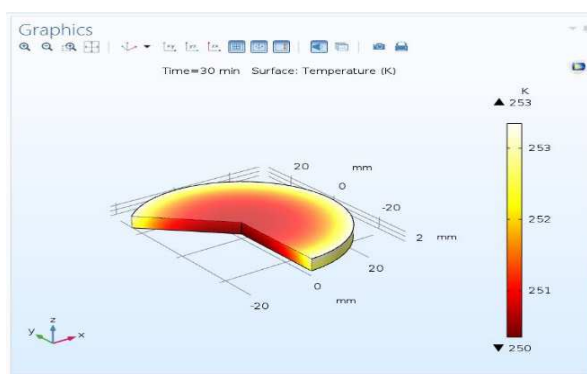


Figure 7: Temperature Distribution after 30 mins

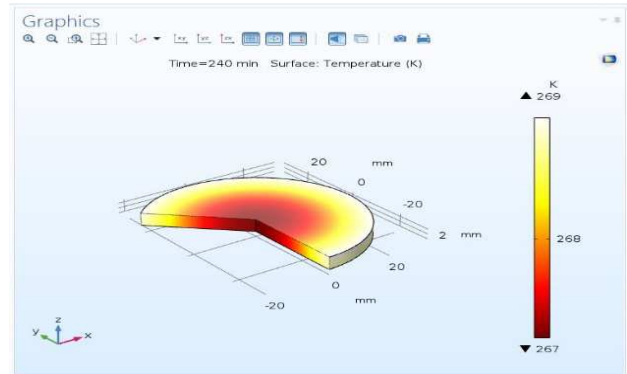


Figure 8: Temperature Distribution after 4 hrs

The figures 7 and 8 show the temperature distribution for an apple slice with the progress of time. Initially, the apple was in frozen state at -25°C , and this model helps to give time required for an apple slice to reach a particular temperature at the central core of the slice. The table 4 shows the time required to get temperature of -15 , -10 , -5°C respectively, at the center of an apple slice.

Table 4: Shows Time Required to Reach Target Temperature

S. No	Temperature ($^{\circ}\text{C}$)	Time (min)
1	-15	80
2	-10	134
3	-5	241

The figure shows the temperature distribution in an apple slice for a time of 400 minutes. This graph clearly shows, the temperature is increasing during the drying stage of an apple slice.

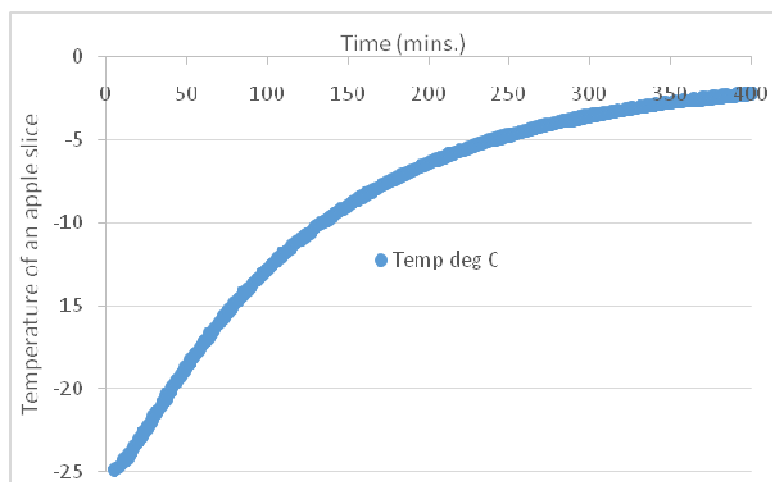


Figure 9: Temperature Distributions in an Apple Slice for a Time of 400 Minutes

5. CONCLUSIONS

In this paper, a model is presented to analyse the behaviour of drying kinetics of an apple slices. The Comsol simulated model predicts the temperature and moisture distribution inside the slice. The moisture distribution of 75%, 50%, 25%, 5% were calculated in the software, which predicts 15, 62, 151, 382 mins respectively, required to achieve the desired moisture content in an apple slice. The simulated results predict the initial model for analysing the temperature and drying kinetics of an apple slice. The computed temperature and theoretical drying kinetics give some confidence in the evolution of the model. Deviations are attributed to thermo-physical variation of the material.

6. ACKNOWLEDGEMENTS

The authors are thankful to CSIR-Central Scientific Instruments Organisation, Chandigarh and National Institute of technical Teachers Training & Research, Chandigarh, for the permissions to use the essential resources, lab equipment and for providing all sorts of facilities required during the course of this research.

REFERENCES

1. Ravník, J. & Golobic, I., "Lyophilization Model of Mannitol Water Solution in a Laboratory Scale Lyophilizer," *Journal of Drug Delivery Science and Technology*, Vol. 45, 2018, pp. 28-38.
2. Datta, A. K., "Status of physics based models in the designing of food products, processes and equipment" *Food Sciences and Food Safety*, Vol. 7, 2008, pp. 121-129.
3. Gan, K. & Bruttini, R., "Freeze drying of pharmaceuticals in vials of trays: Effect of drying chamber wall temperature and tray side on lyophilization performance" *International Journal of Heat and Mass Transfer*, Vol.48, 2005, pp. 1675-1687.
4. Hangos, M. K. & Cameron, T., "Process Modelling and Model Analysis," *Harcourt Science and Technology Company, Academic Press*, 2001.
5. Garg, V. & P. S. Rao, "Heat and Mass transfer Modelling of lyophilization Process for food materials" *International Journal of Technical Innovation in Modern Engineering & Science*, Vol. 5(3), pp. 860-863, 2019.

6. B. Scutella, A. P. Fattori, S. Passot, "3D Mathematical Modelling to Understand a Typical Heat Transfer Observed in Vial Freeze-Drying," *Applied thermal engineering*, Elsevier, pp 226-236, 2017.
7. Pham, Q., "Prediction of calorimetric properties and freezing time of foods from composition data" *Journal of Food Engineering* Vol. 30, 1996, pp. 95-107.
8. Fabiana, R., "Mathematical modelling of drying process of unripe banana slices" *Escola Politecnica of University of Sao Paulo* 2016
9. Stewart, W. & Bird, R., "Transport phenomenon" *John Wiley*, 2002.
10. Kumar, R., Pedgopu, V., Kumar, Anil., Thakur, Robin., & Pundir, Anil. (2013). CFD based analysis heat transfer and friction characteristics of broken multiple rib roughened solar air heater duct. *Int J Mech Prod Eng Res Dev*, 3, 165-172.
11. Otten, L. & Sever, R., "Controlled nucleation in freeze drying: effects on pore size in the dried product layer, mass transfer resistance and primary drying rate" *Journal of pharmaceutical sciences* Vol. 8, 2011, pp. 3453-3470.
12. Perusselo, C. A. & Castilhos, F., "Determination of thermophysical properties of yacon to be used in a finite element simulation" *International Journal of heat and mass transfer* Vol. 67, pp. 1163-1169, 2013.
13. Ramaswamy, H. S. & Tung, M. A., "Thermophysical properties of apple in relation to freezing" *Journal of food science* Vol. 46, 1981, pp. 724-727.